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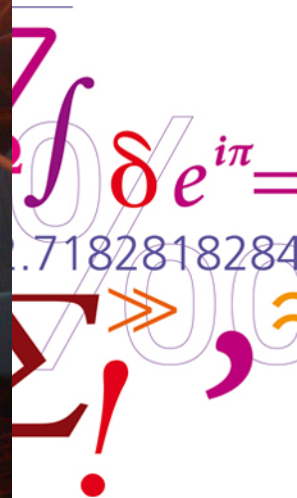
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# High-resolution spectroscopy of gases at elevated temperatures for industrial applications

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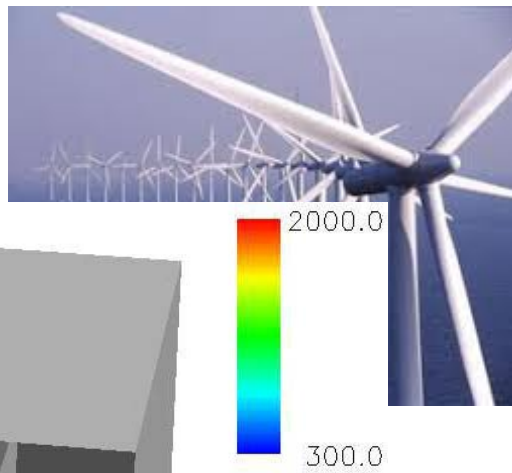


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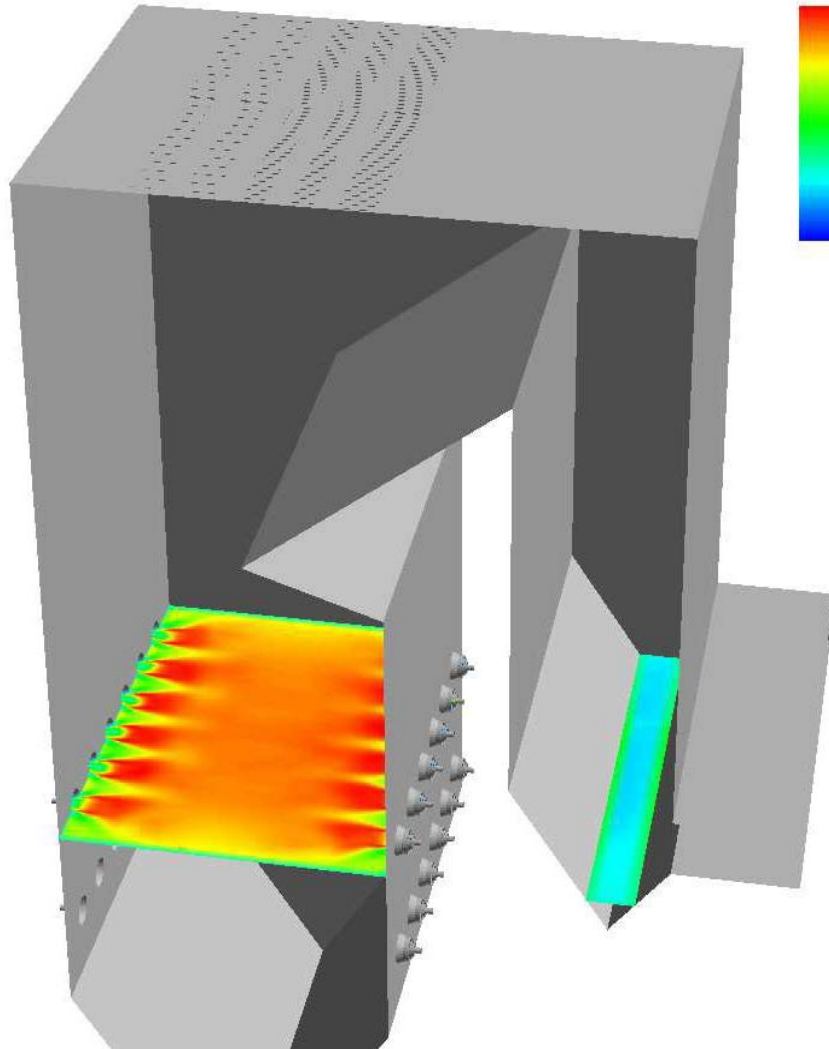
# Outline

- Large scale measurements: why?
- Basic research: how it's made
- High resolution spectroscopy in flow gas cells: H<sub>2</sub>O and CO<sub>2</sub>
- SO<sub>3</sub> project: the story
- Conclusions

# Green Energy...

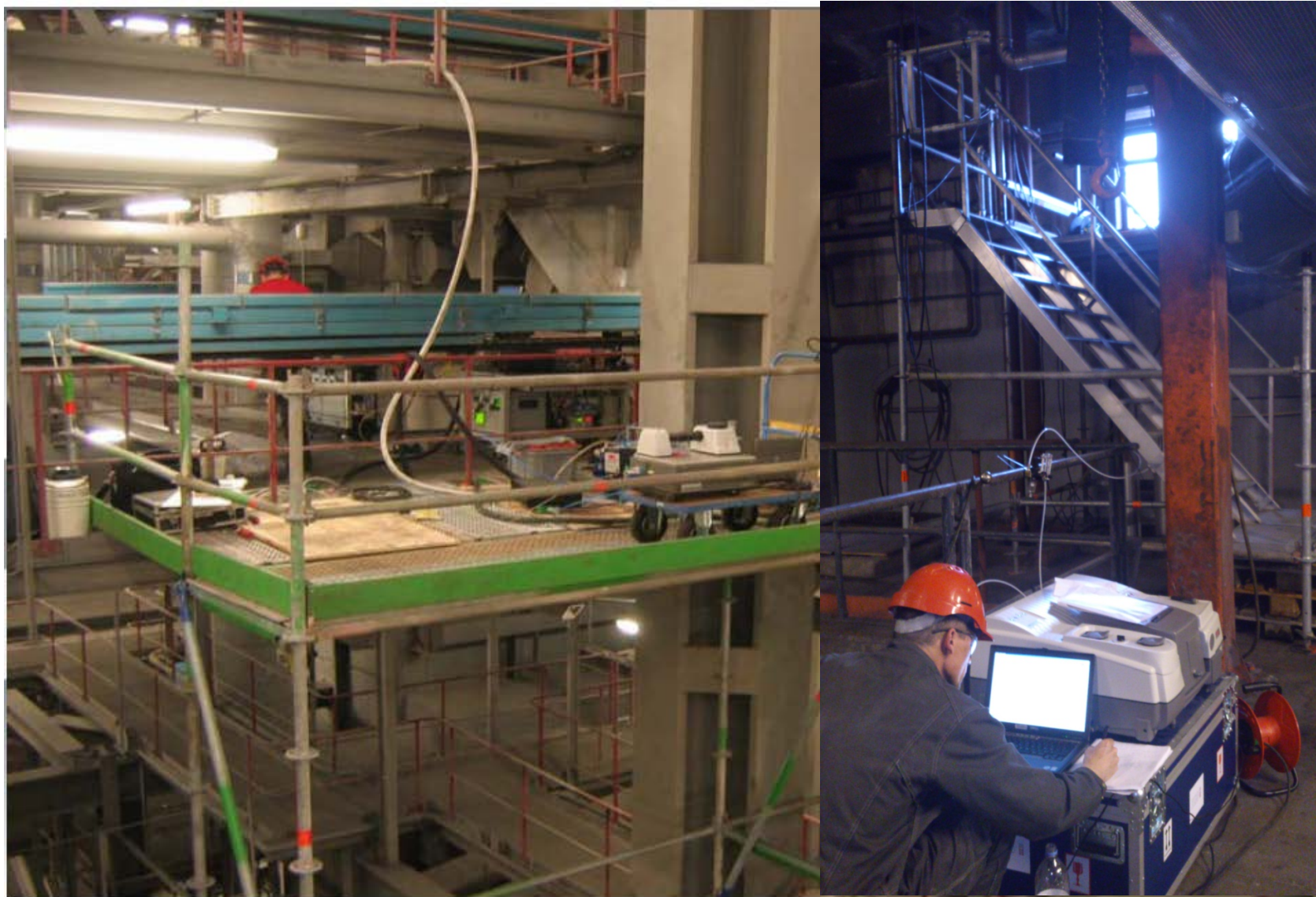


... well





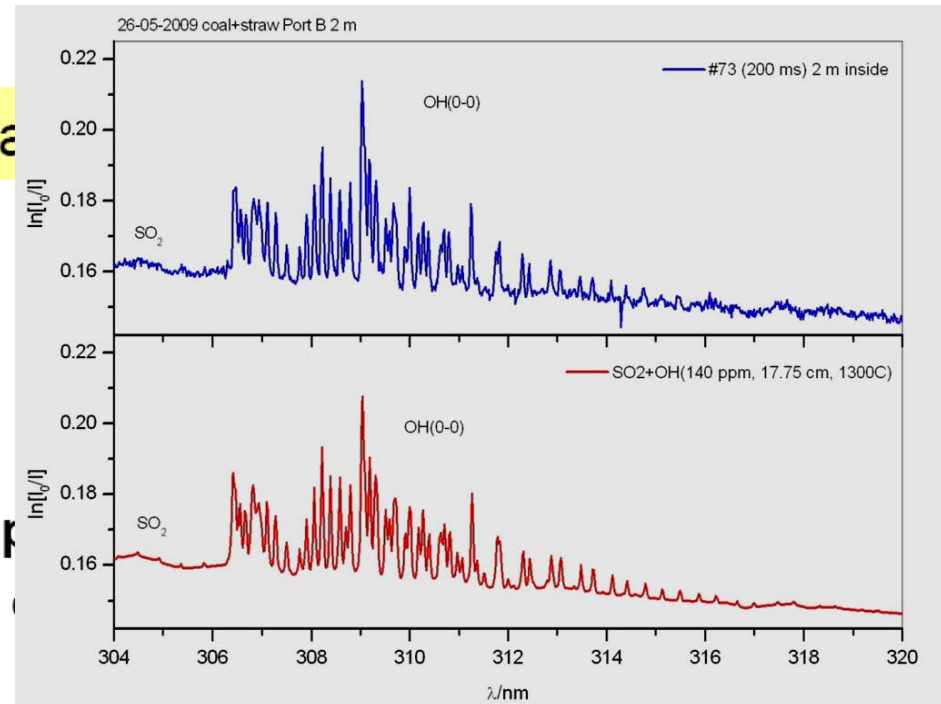
# Large scale measurements



# Large scale measurements

## Fiber optical probes

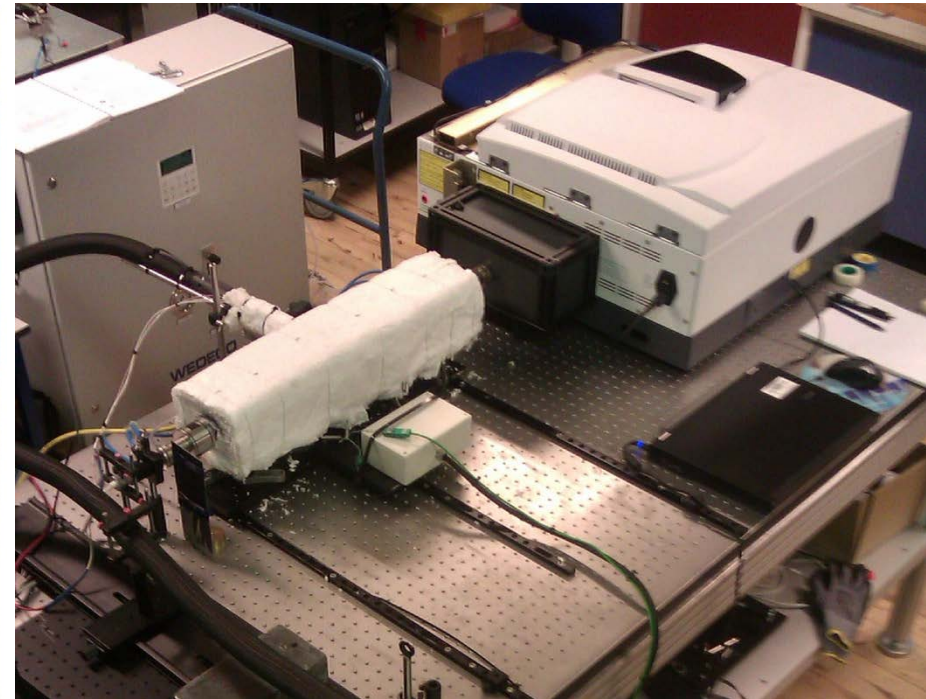
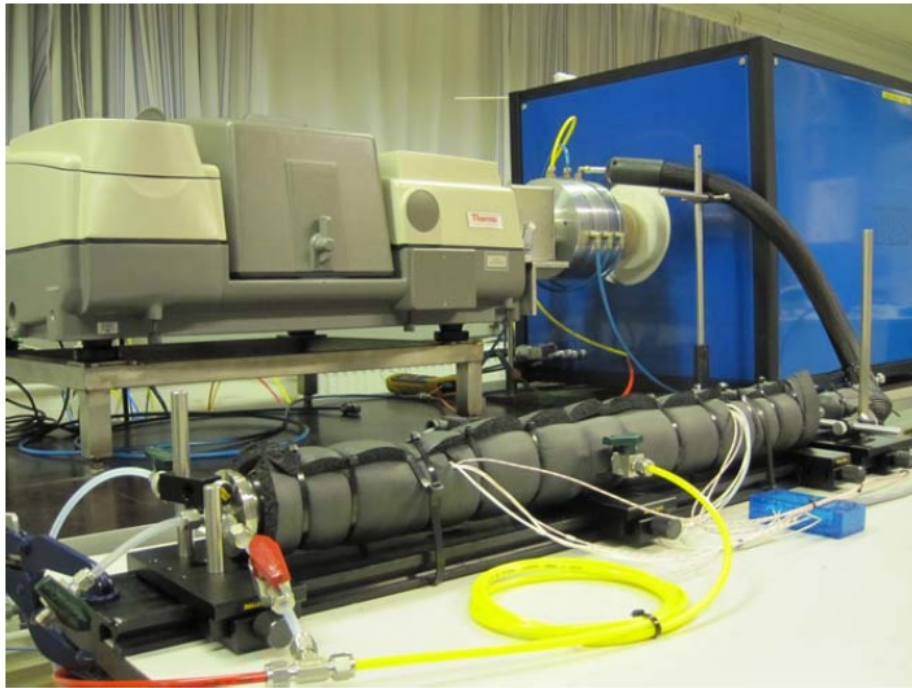
- FTIR spectroscopy (emission): >5 m, 45 mm probe  
 $\text{H}_2\text{O}$ ,  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{C}_x\text{H}_y$ ,  $\text{HCl}$ , etc. +  $T_{\text{gas}}$  +  $T_{\text{par}}$  +  $\epsilon$
- UV spectroscopy (transmission): 9 m, 60 mm probe  
 $\text{SO}_2$ ,  $\text{NO}$ ,  $\text{O}_2$ , etc.





# Basic research

- focus on optical properties (TRS, ABS) of gases at temperatures up to 1600C;
- validation/building databases (e.g. HITRAN/HITEMP/CDSD...);
- high-resolution spectroscopy ( $0.125\text{ cm}^{-1}/0.016\text{ nm}$ ) of “major” and “minor” (or trace) gases : [CO<sub>2</sub>](#), [H<sub>2</sub>O](#), [SO<sub>2</sub>](#), [NH<sub>3</sub>](#), [SO<sub>3</sub>](#), [H<sub>2</sub>S](#), [OCS](#), [HCL](#), [CH<sub>3</sub>Cl](#), [PAH's](#) etc;
- various hot gas cells with highly-uniform temperature profiles ( $\pm 0.5\text{C}$ ).

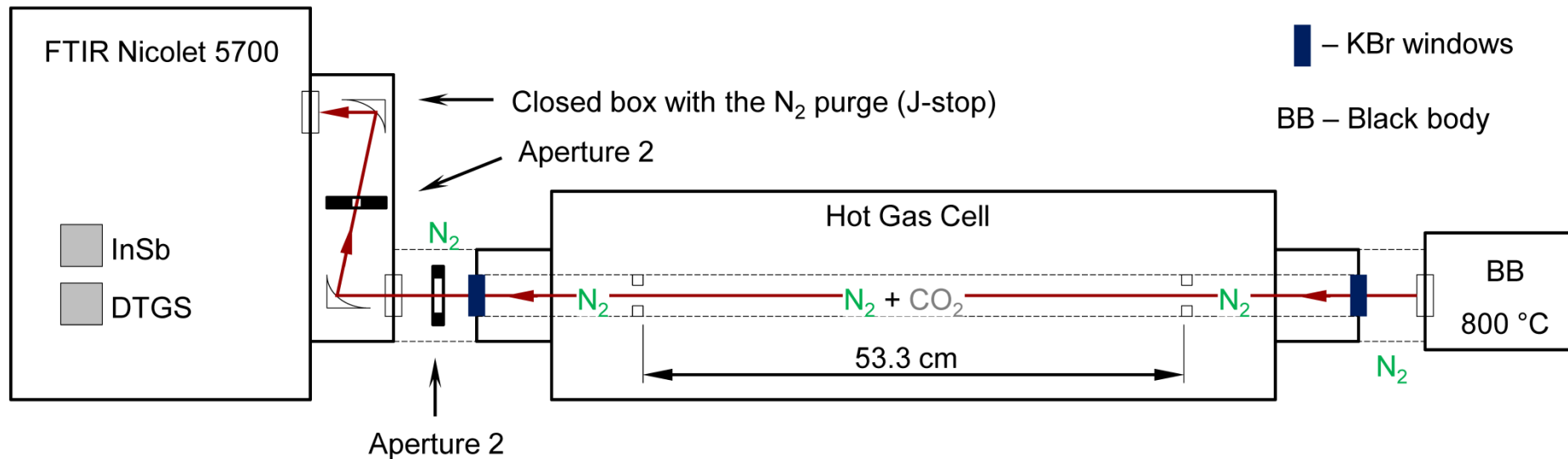


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# Experimental set up

Includes:

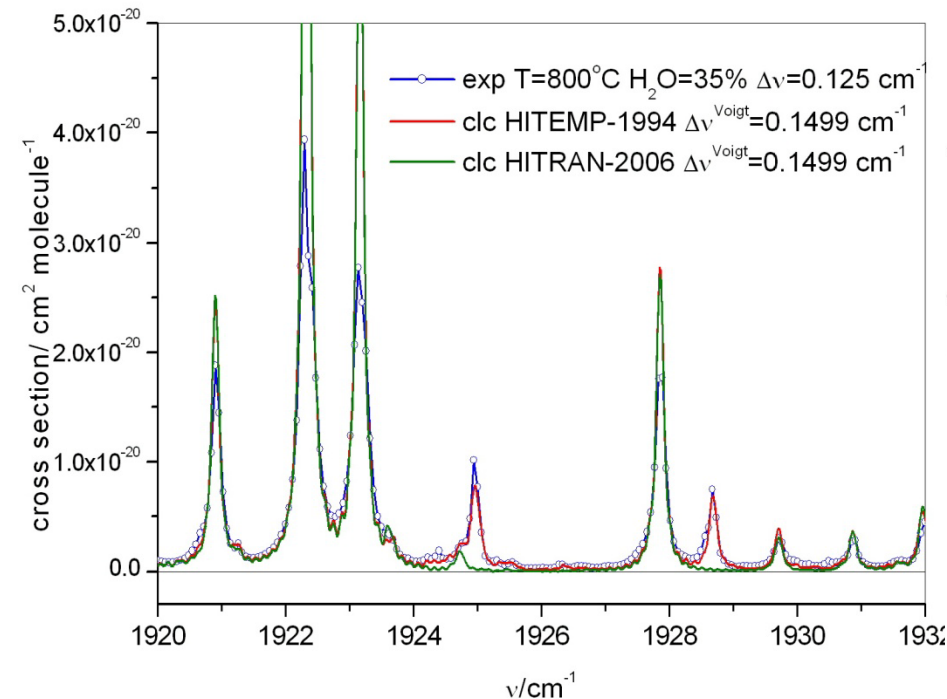
- a gas cell;
- a high-resolution FTIR spectrometer (Nicolet or Agilent);
- a light source (BB).



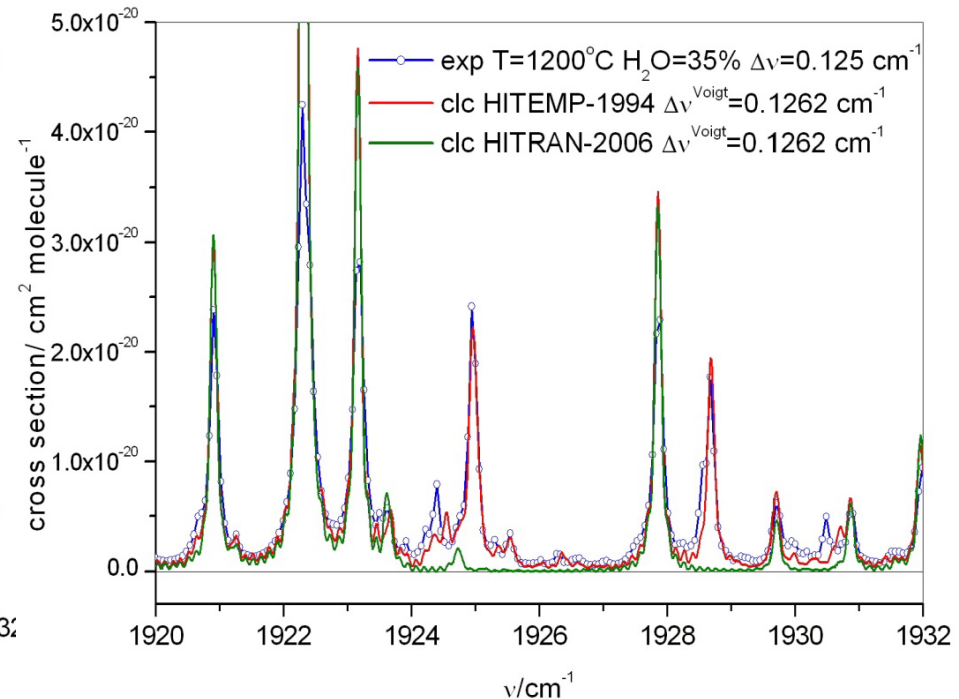


# Examples: H<sub>2</sub>O absorption cross sections

T=800C

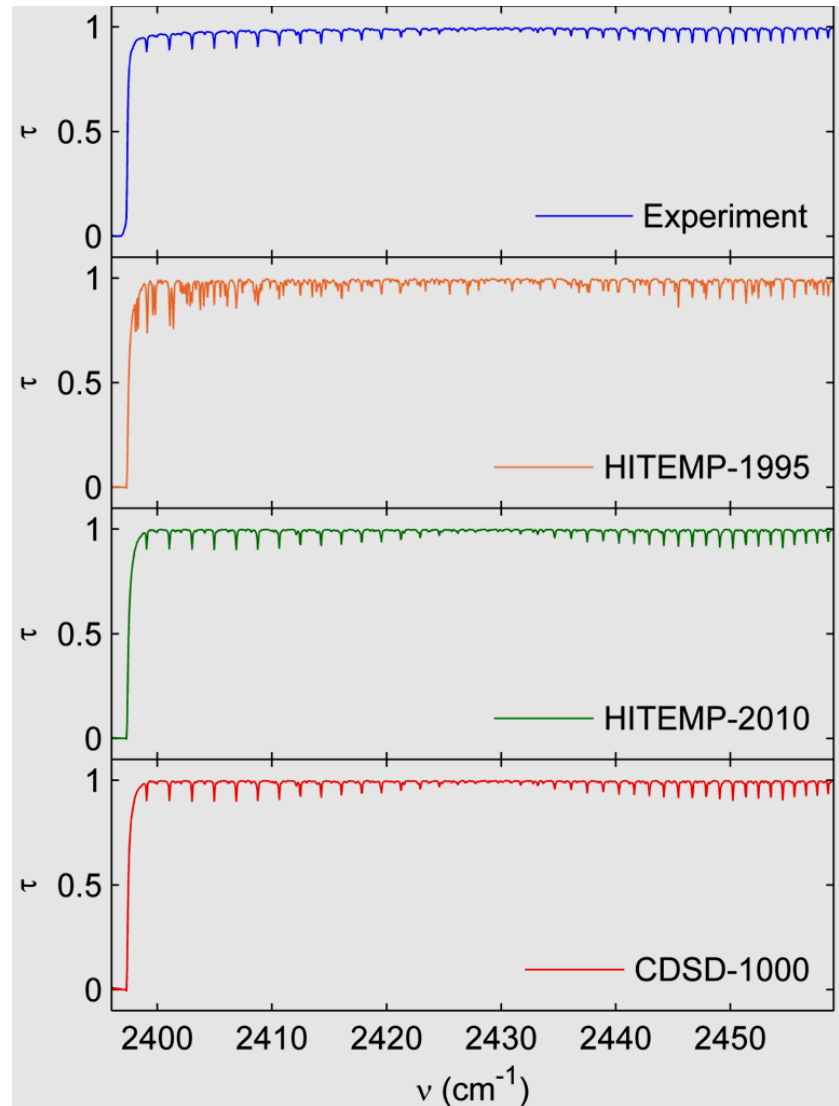
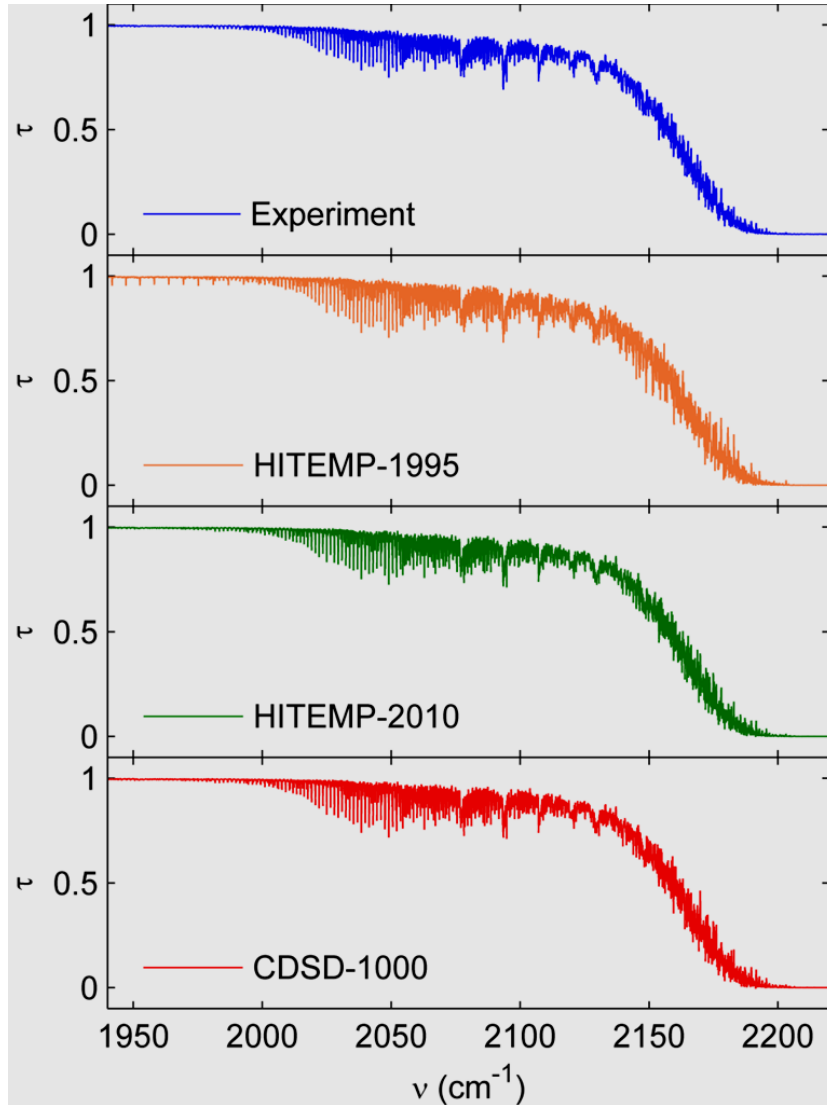


T=1200C

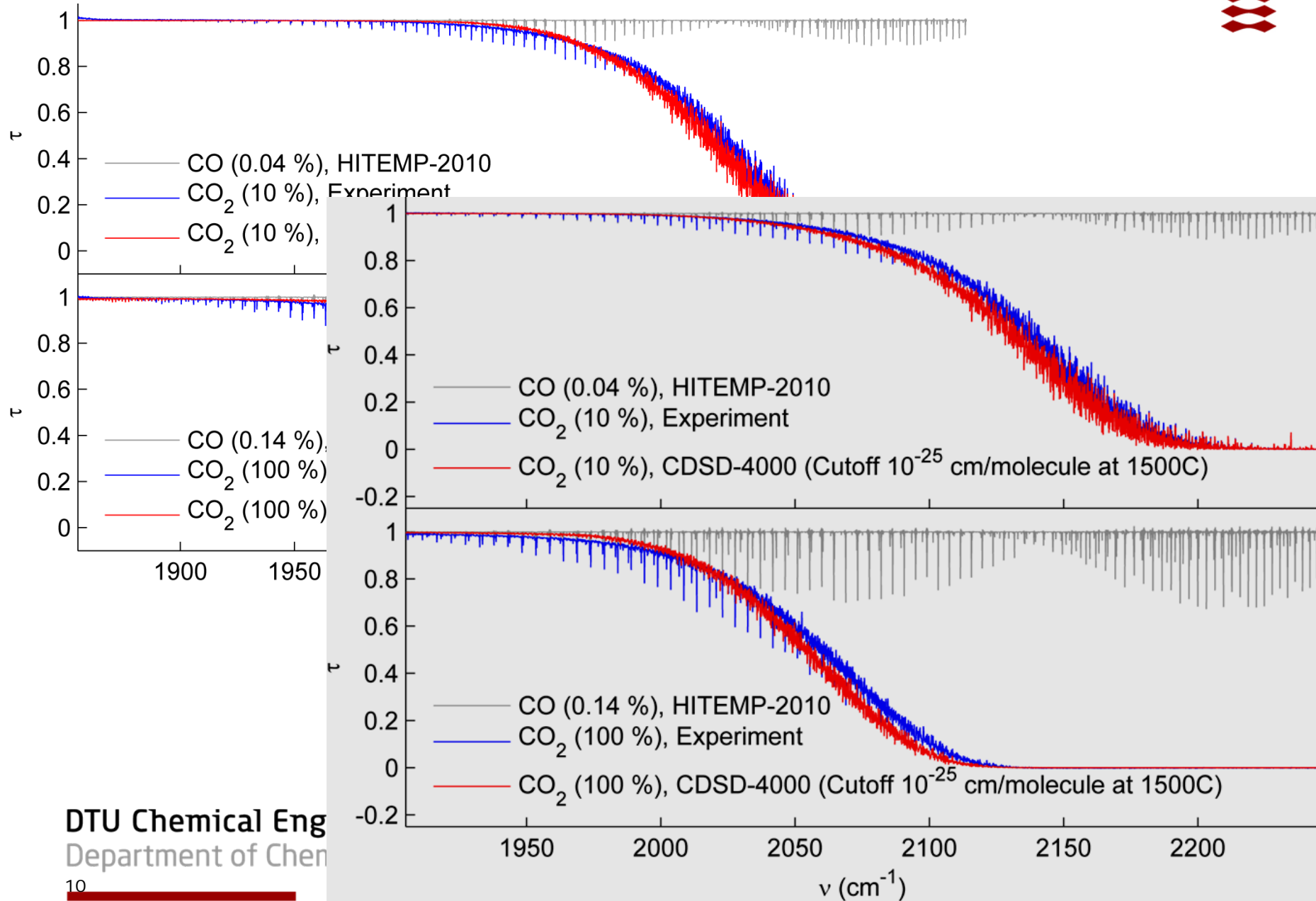


- Good agreement between EXP and CLC(HITEMP-1994);
- Different FWHM values of the H<sub>2</sub>O single lines for H<sub>2</sub>O(35%) in N<sub>2</sub> and H<sub>2</sub>O(35%) in CO<sub>2</sub> (oxyfuel combustion).

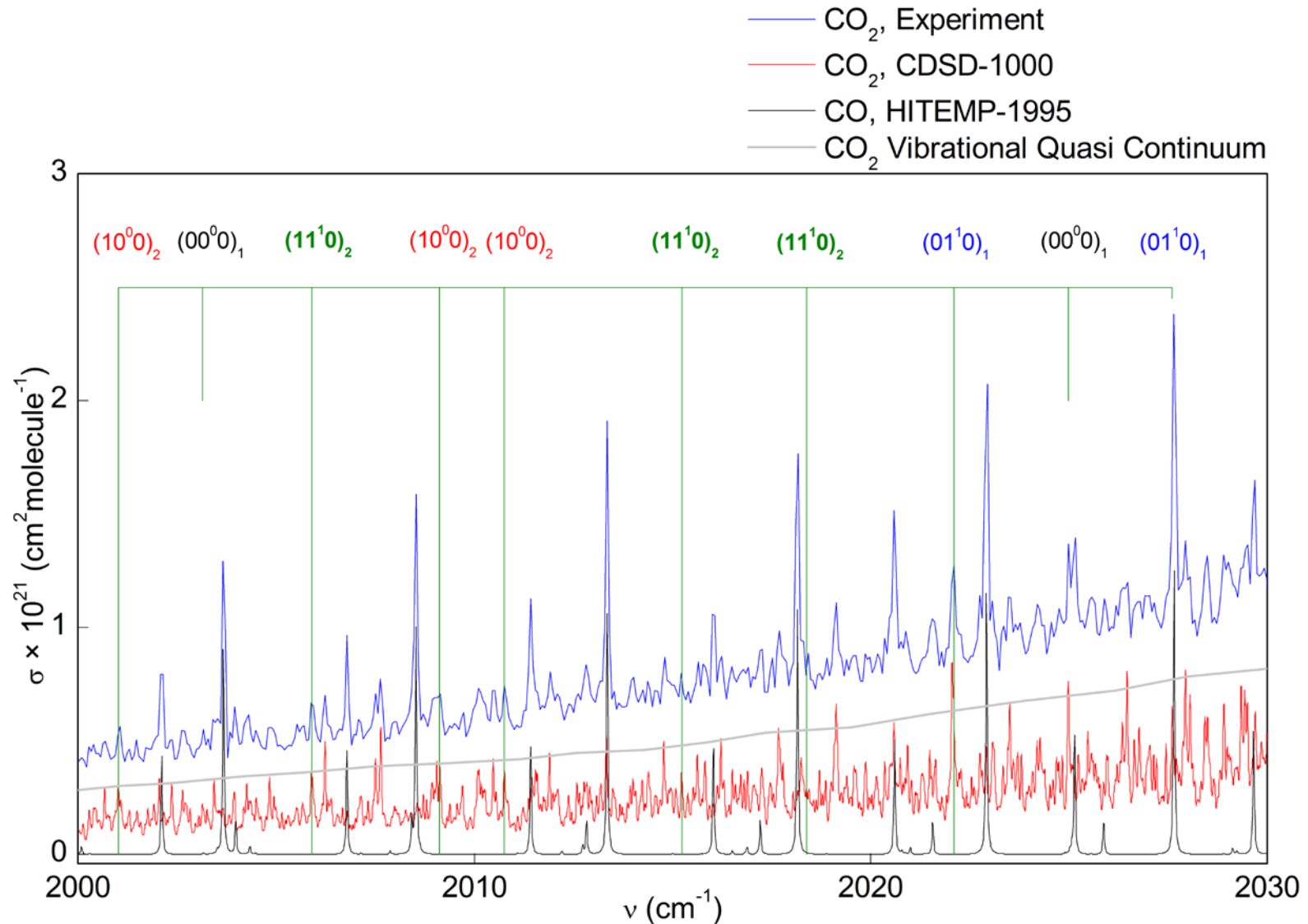
# CO2 transmission spectra: 727C



# CO<sub>2</sub> transmission spectra: 1500C

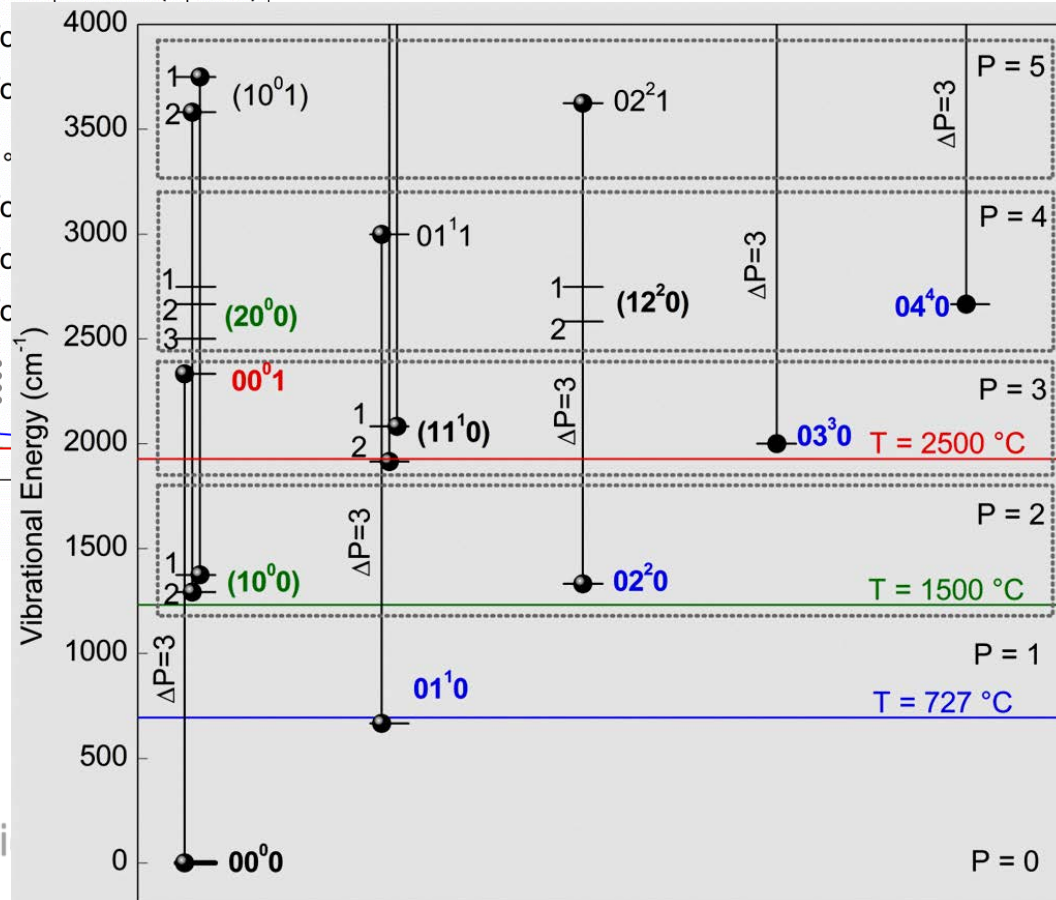
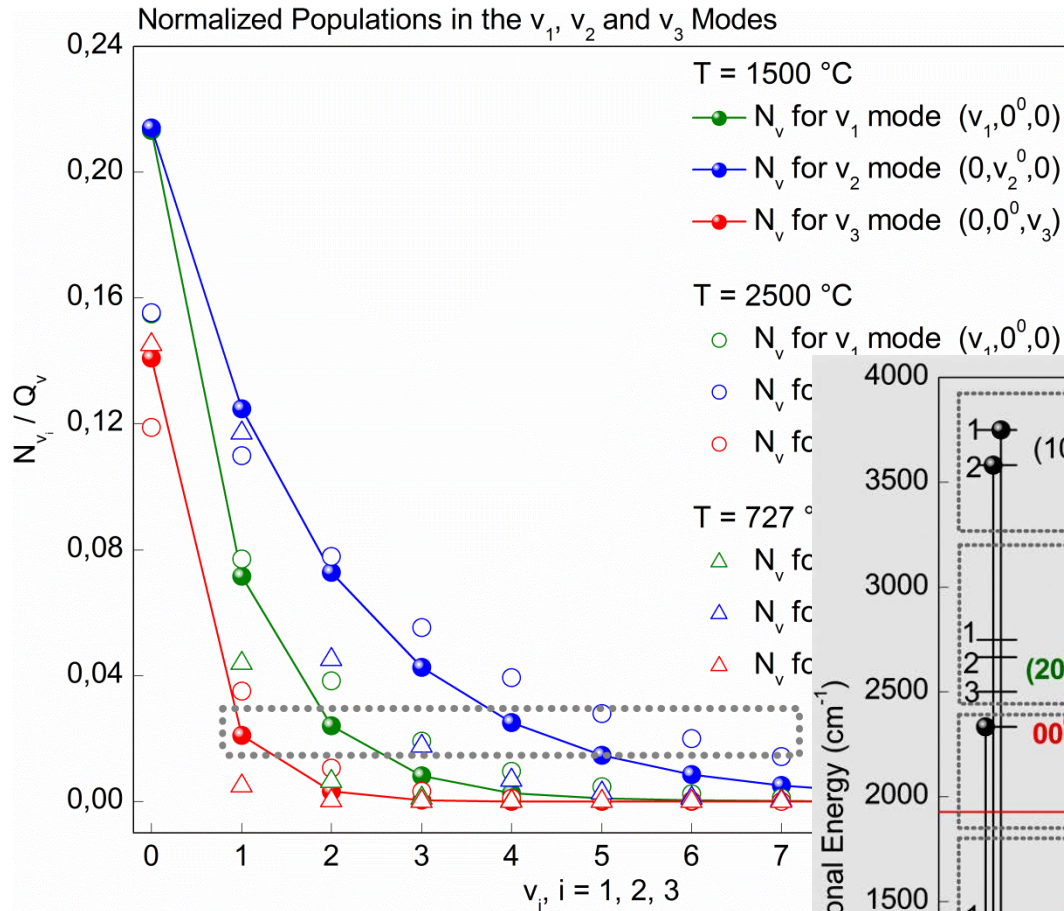


# CO<sub>2</sub> quasicontinuum at 1500C





# CO<sub>2</sub> quasicontinuum at 1500°C



# SO3 project: industry and university

## Facts:

- Coal air combustion: SO<sub>2</sub>(300ppm) and SO<sub>3</sub>(5ppm) (blue smog);
- Large power plants: SCR units (NO<sub>x</sub> reduction) with NH<sub>3</sub> injection;
- Global warming: operation at lower loads;
- Lower loads: lower gas temperatures at SCR units;
- By law: not allowed to turn off NH<sub>3</sub> injection system.

## Problems:

- Non optimal NH<sub>3</sub> consumption;
- At lower T: H<sub>2</sub>SO<sub>4</sub> formation which causes ammonia sulfate and ammonia bisulfate formation;

## Consequences:

corrosion in ducts and plugging/damage of SCR elements.

## Goal:

to develop an optical method for SO<sub>3</sub> *in situ* measurements.

# SO3 project: industry and university

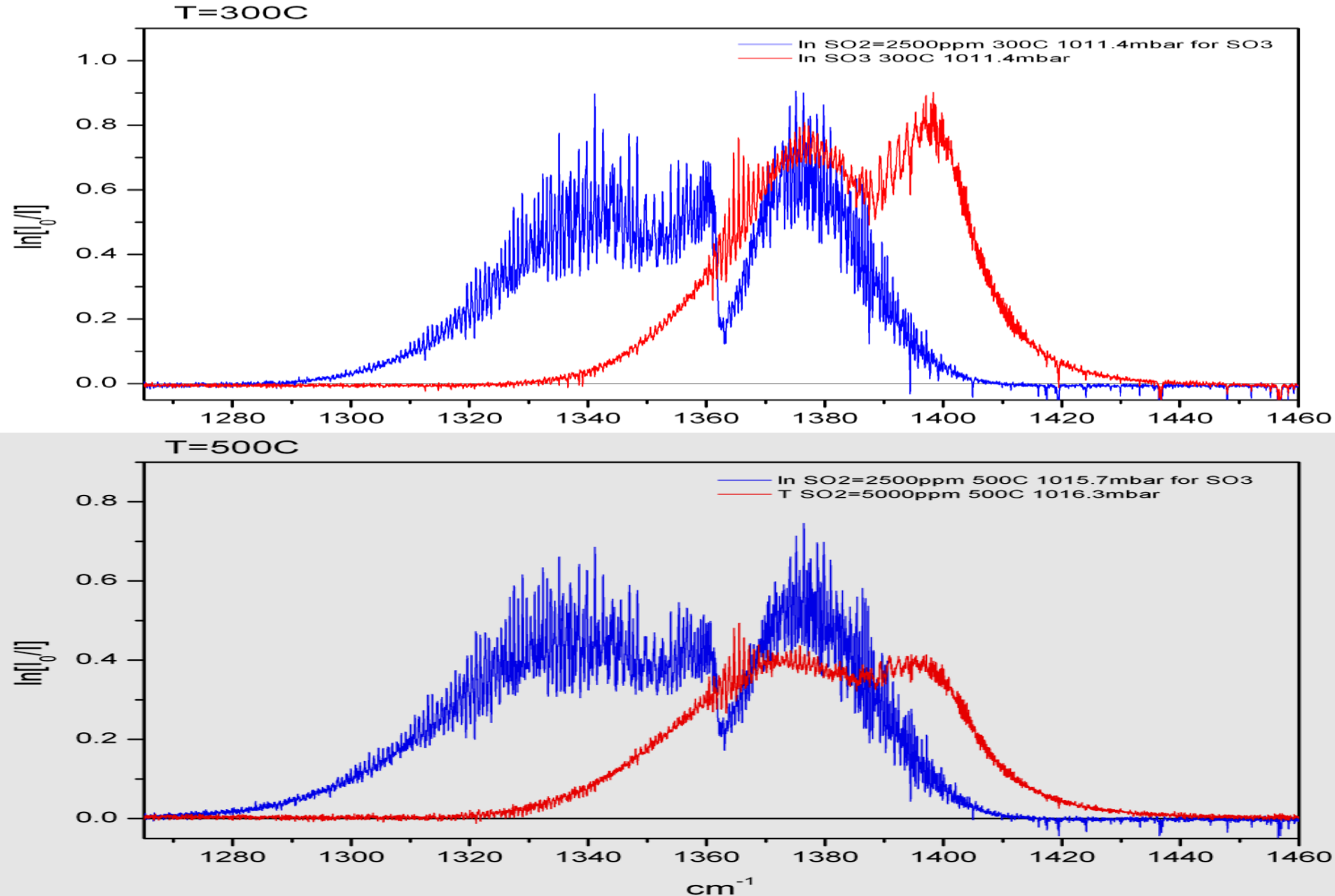
Challenges of the project:

- temperature range 200-500C;
- SO3 high-resolution spectra (SO3 generation);
- SO2, NH3, H2SO4 and H2O high-resolution spectra database;
- water cooled optical probe development;
- powerful IR light source development;
- high sensitivity FTIR with linearized MCT or InSb detector;
- use of modern mathematical tools (e.g. SVD, NNLS).

Two phases of the project:

- measurements in the lab and SO2/SO3 line list generation (UCL, UK)
- measurements on an industrial scale (power plant, Dong Energy, DK)

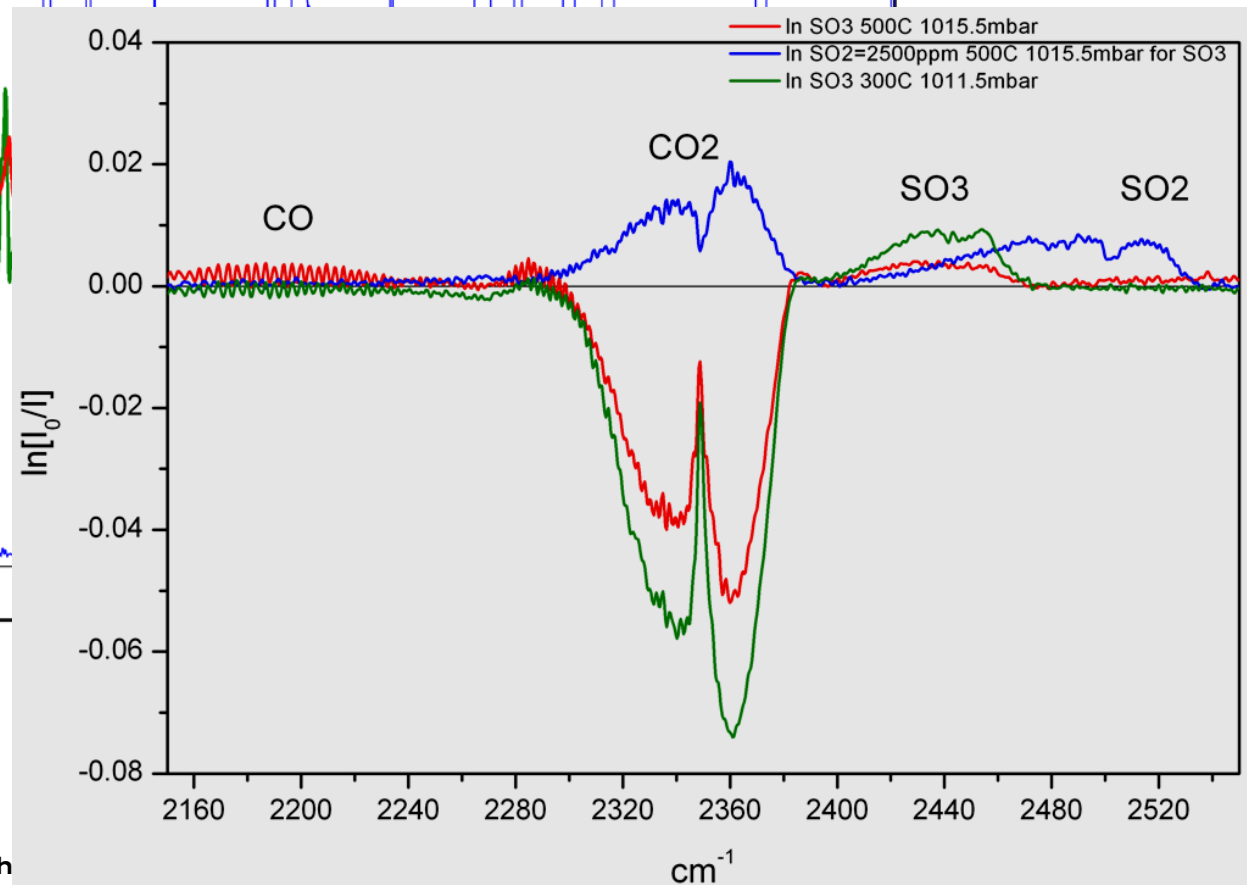
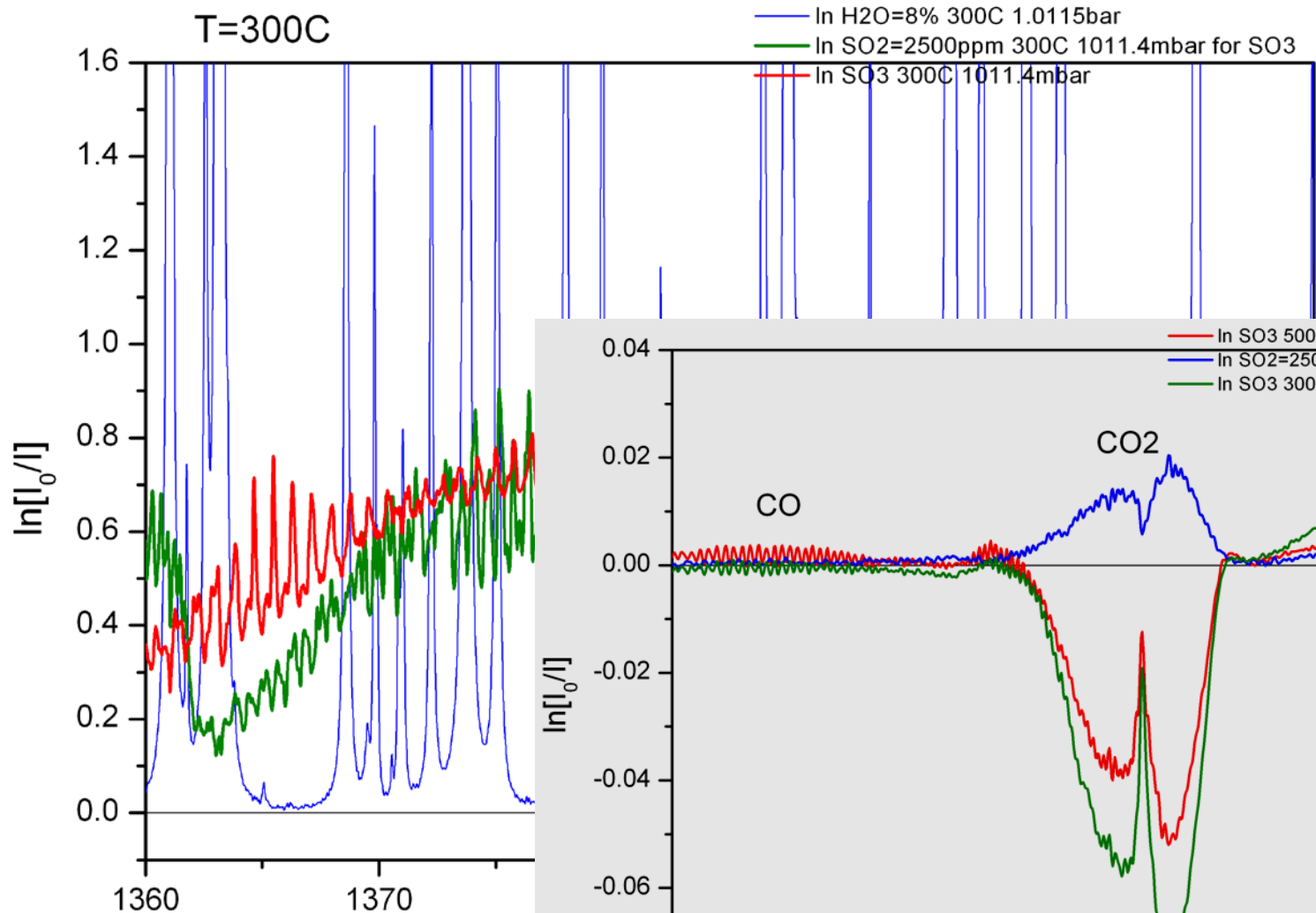
# SO3 project: high-resolution (0.115 cm<sup>-1</sup>) measurements





# SO3 project: interferences

T=300C



# Conclusions

High quality optical measurements with various gases (incl. highly corrosive gases) are possible;

A new gas cell is under development ( $<200$  bar,  $2000^{\circ}\text{C}$ )

Measurements can be used for: databases development and validation, studies of chemical reactions, energy exchange, validation of line shape models.

SO3 project is under development: lab work + PhD student employed by UCL;



# Acknowledgements

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- UCL (Prof. Jonathan Tennyson)